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Benchmarking Exchange-Correlation Functionals in Density Functional Theory (DFT) using Experimental Compton Profiles

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Abstract
The process of benchmarking exchange–correlation (XC) functionals presents a significant challenge to Density Functional Theory (DFT) because the accuracy of these functionals determines how reliably electronic structure calculations produce results. The research uses experimental Compton profiles as a momentum-resolved standard to determine how well common exchange-correlation functionals perform in practice. Researchers conduct a detailed comparison between high-quality experimental Compton scattering data and theoretical profiles which DFT calculations produce using local, semilocal, and hybrid functionals. The study shows that all functionals can reproduce the basic features of experimental profiles yet there exists a substantial gap between their results and actual experimental data particularly in areas where electrons become localized and form chemical bonds. Valence electrons tend to be over-delocalized by local density approximations while experimental results show better agreement with generalized gradient and hybrid functionals. The findings demonstrate how Compton profiles react differently to small XC estimation errors which serves as a secondary benchmark method that extends beyond standard energy measurements and provides guidance for future functional development and validation.

Keywords: *Exchange–Correlation, Density Functional Theory, DFT Calculations, XC Estimation, Compton Profiles etc.*

I. Introduction

1.1 Density Functional Theory and the Central Role of Exchange–Correlation Functionals

Theoretical framework of Density Functional Theory (DFT) serves as the most common method for studying electronic structures in atomic, molecular, and condensed matter systems. The method achieves its scientific importance because it delivers accurate results through efficient calculations which researchers utilize in physics, chemistry, and materials science work. DFT uses electron density functionals to model total energy systems as it transforms complex many-electron systems into simpler single-particle systems (Hohenberg & Kohn, 1964). DFT establishes a formal foundation which proves that mappings exist, yet DFT calculations require specific XC functional selection to achieve practical accuracy. The XC functional describes all many-body effects that happen because of electron-electron interactions, which the classical Coulomb term does not capture, and it stands as the only uncontrolled approximation that exists in standard DFT.

The exchange-correlation functional is the only uncontrolled approximation in standard density functional theory (DFT). It includes all of the many-body effects that the standard Hartree term doesn't take into account, such as electron exchange (which is based on the Pauli exclusion principle) and electron correlation (which is based on Coulomb interactions). Researchers typically navigate this process utilizing a hierarchical structure known as "Jacob's Ladder," progressing from the Local Density Approximation (LDA) to Generalized Gradient Approximations (GGAs), and eventually to more advanced hybrid functionals.

Over the decades, scientists developed various XC functionals which form a hierarchical structure that starts with local density approximation (LDA) and progresses to generalized gradient approximations (GGAs), meta-GGAs, and hybrid functionals (Kohn & Sham, 1965). Each class attempts to include more advanced physical data about electronic systems, which includes density gradients and kinetic energy density and a portion of exact exchange (Perdew et al., 1996). No XC functional exists which can accurately predict every material property across all types of materials despite their widespread adoption. The process of systematized benchmarking requires researchers to compare different functionals against trustworthy experimental data because this method helps determine functional strengths and weaknesses and informs the creation of better approximation methods.

1.2Experimental Probes of Electron Momentum Density

The standard tests for XC functionals use basic physical attributes which include lattice parameters and binding energies and material strength and electronic energy gaps. The electronic structure of materials can be investigated through these measurements because they show various features of material properties which scientists can use to understand material behavior. The experimental methods which directly measure electron momentum density provide scientists with a more accurate method to evaluate theoretical models. High-energy Compton scattering stands out among these methods because it provides scientists with a special way to conduct research.

Compton scattering experiments measure the inelastic scattering of high-energy photons by electrons in a material which provides access to the Compton profile that shows the ground-state electron momentum density in one-dimensional format. Compton scattering provides bulk-level measurement abilities which remain mostly unaffected by surface factors unlike most spectroscopic methods exchange (Perdew et al., 1996). The impulse approximation which operates at high photon energy levels permits the measurement of Compton profiles to show fundamental ground-state characteristics without showing any final-state effects. The experimental Compton profiles obtained from measurements provide scientists with a strong reference point to compare their theoretical predictions of electron momentum distributions which they calculate using DFT methods.

1.3 Motivation for Benchmarking XC Functionals Using Compton Profiles

Compton profiles show high sensitivity to electronic wavefunction details which makes them useful for testing XC functionals in total-energy measurements beyond standard benchmarks. The Compton profile shows different shapes and anisotropy patterns between low and intermediate momentum ranges because of exchange and correlation differences that scientists use to create their measurement systems. The experimental comparison between Compton profiles & DFT predictions helps scientists understand the process how well different functionals can simulate solid-state electron behavior. Scientists have put more research effort into energy-based benchmarks than they have into testing XC functionals with Compton scattering data for benchmarking purposes (Cooper et al., 2004). The existing studies use particular materials and a limited number of functionals which makes it impossible to reach universal conclusions. The progress made in experimental resolution and computational techniques provides researchers with better tools for precise comparisons between their current work and previous studies from earlier decades. High-quality experimental Compton profiles create an opportunity for researchers to conduct a complete and critical evaluation of XC functionals in their assessment.

1.4 Scope and Objectives of the Present Study

The current research work plans to perform systematic testing of common exchange–correlation DFT functionals through experimental results which they will compare to theoretical Compton profiles (Bansil et al., 1999). The study evaluates different functionals according to their ability to replicate quantum-mechanical electron behavior in solids through its examination of electron momentum densities instead of total energy measurements. The analysis examines both the experimental match results and the momentum-dependent discrepancies which originate from particular XC functional approximation methods. The research study demonstrates how present-day DFT functionals function while showing Compton scattering as an effective benchmark tool which scientists use too little to test electronic structure theories.

1.5 Novelty Statement

This study provides a comprehensive benchmarking of contemporary functionals, including meta-GGAs and range-separated hybrids, against high-resolution synchrotron data (0.1 a.u. resolution), unlike previous studies that focused on particular materials or restricted functional sets. We introduce a multi-region performance metric that evaluates accuracy separately for valence-dominated (low-momentum) and core-dominated (high-momentum) regions, enabling a more nuanced analysis of XC errors than the traditional Mean Absolute Deviation (MAD).

II. Theoretical Background

2.1 Background in Density Functional Theory

Density Functional Theory establishes a complete framework for analyzing many-electron systems through its approach which uses electron density as the fundamental variable instead of the complete many-body wavefunction. The Hohenberg–Kohn theorems show that the ground-state electron density serves as the sole determinant for all system properties which include external potential and total energy thus establishing the framework for density functional theory (DFT) (Levy, 1979). The Kohn–Sham method creates an equivalent system which contains non-interacting electrons that travel through a constructed effective potential. The effective potential combines the external nuclear potential with the Hartree term which describes electron–

electron Coulomb repulsion and the exchange–correlation potential which handles all remaining many-body effects. The field of electronic property prediction requires precise results about exchange–correlation functional because its exact characteristics remain unknown.

Solving self-consistent one-electron equations produces single-particle orbitals that constitute the ground-state electron density inside the Kohn–Sham framework (Parr & Yang, 1989). The artificiality of these orbitals does not prevent their ability to accurately represent electronic structure which makes them a popular tool for studying experimental results. The exchange–correlation functional determines how electron density develops together with its associated momentum distribution patterns. The ability to predict electronic structure results requires researchers to understand how different functionals affect electronic wavefunctions because this knowledge helps them evaluate functional performance through comparison with direct electronic structure research.

2.2 Hierarchy of Exchange–Correlation Functions

The main method for solving physical problems through DFT studies uses exchange-correlation functionals. The method uses Coulomb forces to model how electrons move and it uses Pauli exclusion to simulate the process of electron exchange. The local density approximation uses electron density measurements from all regions in a system to determine exchange-correlation energy which represents the most basic modeling approach. The density operates as an electron gas that occupies all available space (Perdew et al., 2009). The LDA method proves effective for various materials because it generates multiple bonds but fails to capture uneven electron distribution. Generalized gradient approximations provide superior descriptions of covalent and ionic solids compared to LDA because they combine local density data with information about spatial gradient changes. Meta-generalized gradient approximations, which depend on the kinetic energy density or density Laplacian, capture more subtle electronic structural properties. Hybrid functionals represent an essential group of methods which combine exact exchange from Hartree–Fock theory with additional operational rules for implementing hybrid interface functional methods (Becke, 1996). DFT relies on exchange–correlation functionals for two functions which include electron exchange modeling based on the Pauli exclusion principle and electron correlation modeling through Coulomb interaction effects. The local density approximation, which represents the most basic modeling approach, defines exchange–correlation energy based on local electron density at every spatial point, which behaves like an electron gas that exists uniformly throughout space. The LDA method effectively predicts metal and various other material behavior patterns, yet it generates excessive binding results when applied to semilocal correlation functionals in single-electron calculations. The hybrid approach increases band gap values whereas it enhances molecular characteristics but scientists must conduct additional research to understand hybrid performance during momentum transitions, which serves as a crucial testing standard. Hybrid functionals function as essential computational tools because they combine exact exchange from Hartree-Fock theory with semilocal correlation functionals. Researchers still don't know how these functions work with different momentum, which makes evaluating them very difficult. Hybrid functions improve band gap and molecular features.

2.3 Solid electron momentum density

Electron momentum density defines the distribution of electrons in momentum space and supplements the electron density in actual space. The momentum density derives from the one-particle density matrix through its Fourier transform, which connects to the electronic wavefunctions that quantum mechanics considers to be occupied. The momentum density of crystalline solids demonstrates how electron localization and hybridization and correlation effects determine which lattice patterns and chemical bonds exist (Singh & Nordström, 2006).

In independent-particle approximation the total momentum density of the system results from summing all Kohn-Sham orbitals that are currently occupied. The exchange-correlation functional contains many-body effects because it includes electron-electron correlations which our approximation does not include (Mijnarends&Singru, 1974). Theoretical and experimental momentum density discrepancies emerge because functional restrictions create limitations on calculations. Kohn-Sham orbital spatial arrangements change when different exchange-correlation approximations are applied which affects their momentum space Fourier-transformed versions and leads to separate momentum density patterns.

2.4 Momentum Density Projections from Compton Profiles

Scientists use Compton scattering experiments to obtain Compton profiles which allow them to measure the momentum density of electrons. The process of converting Compton profiles from three-dimensional momentum density data allows scientists to obtain one-dimensional results which display momentum density along the scattering vector direction. The impulse approximation at high photon energy works because it requires only the electron ground-state momentum distribution without needing final-state

interaction or multiple scattering effect data (Bansil &Mijnarends, 1989). Theoretical computations can be validated through experiments because Compton profiles serve as dependable experimental measurements.

Theoretical calculations of Compton profiles require DFT momentum density to be integrated across all momentum components which move perpendicular to the scattering vector. Low and intermediate momentum regions of the profiles experience high sensitivity because exchange and correlation effects control these areas (Sakurai & Itou, 2004). The Compton profile's shape and directional distribution become distorted through electronic wavefunction imperfections which remain hidden during total-energy assessments. Compton scattering enables researchers to conduct precise evaluations of exchange-correlation functionals through its clear physical framework which links theoretical methods to measurable experimental results while establishing a foundation for comprehensive benchmarking studies.

III. Review of Related Literature

The process of testing exchange–correlation functionals which exist within Density Functional Theory through experimental Compton profiles establishes an unique interdisciplinary field which connects electronic structure theory with momentum-space observables and experimental scattering physics. Researchers have studied Compton scattering experiments for decades comparing their results to theoretical predictions which different DFT functionals and computational models generated. The experiments demonstrate new research methods yet they reveal ongoing challenges which scientists face when trying to measure electron momentum concentrations found in materials.

Researchers have dedicated their studies to directly comparing experimental Compton profiles with theoretical calculations which model simple metals. In their initial high-resolution Compton scattering study of aluminum***Ohata et al. (2000)*** tracked directional Compton profiles and compared those profiles to profiles created through the local-density approximation (LDA) method. The results exhibited a strong agreement between profile shape and anisotropies, but the results showed major differences between low momentum points and profile tail sections which proved that LDA cannot accurately depict electron correlation effects during momentum space analysis. The LDA exchange and correlation handling problems caused these inconsistencies, which LDA used to calculate total energies and bulk properties yet failed to capture momentum-dependent characteristics at a detailed level.

Researchers have used Compton profiles from beryllium, aluminum, and titanium elemental systems to test generalized gradient approximations (GGAs) through their experimental Compton profiles. ***The Journal of Physics and Chemistry of Solids published a comparison study which examined isotropic profiles of Be, Al, and Ti (2013)*** by comparing theoretical GGA-based momentum densities with high-energy experimental data that extended to 9 atomic units of momentum transfer. The studies demonstrated generally satisfactory concordance, particularly in intermediate momentum regions, while the ongoing discrepancies at low momentum showed how semilocal functionals differ in their ability to model valence electron distribution patterns.

The studies about metals show that semilocal functionals which include LDA and GGAs achieve acceptable results for standard Compton profile measurements but fail to represent complex momentum-space behavior which depends on the specific exchange-correlation approximation used. The research team studied advanced materials which included ***α- and β-phase GeTe (2011)*** by using Compton profiles together with band structure simulations to investigate how momentum density correlated with electronic topology near the Fermi level. The extended gradient approximation in that study provided results more aligned with experimental data than the local density approximation, highlighting the significance of gradient corrections in accurately depicting electron distributions associated with bonding and hybridization.

The recent studies have expanded their research scope to include testing more advanced chemical compounds together with hybrid functional measurement methods. The research study on TiSXTe (M = Ti Zr) compounds introduced the first Compton profiles for these materials which were compared with experimental data through theoretical calculations that used hybrid exchange-correlation approximation methods and traditional hybrid methods like PBE0 and B3PW. The findings demonstrated that hybrid functionals deliver better accuracy for predicting momentum densities and electronic responses than standard semilocal approximations.

The research of electronic structure theory methodological studies together with their selected materials shows how different methods impact their functional performance results. ***Mali et al. (2022)***other researchers proved that present exchange-correlation functionals fail to deliver accurate electron density results. Highly parametrized functionals show excellent total energy results for atoms and small molecules. The energy standards do not provide sufficient accuracy because the system produces inconsistent density forecast results. The research shows that solids exhibit the same pattern from the study. The study ***Assessing Exchange–Correlation Functionals for Accurate Densities of Solids (2024)*** shows that a functional can produce accurate lattice constants and cohesive energies but will not achieve correct momentum-space observable results.

Researchers have used Compton profiles to study how electrons interact with each other in ways that exceed the limits of standard DFT. The study ***Inelastic Compton scattering (2023)*** shows researchers used DFT together with dynamic mean-field theory (DMFT) to investigate magnetic Compton profiles in ferromagnetic Fe and Ni. The study shows how electronic correlations change with different momentum space processes. The dynamic correlation inclusion through DMFT modeling enhances experimental results alignment when compared against standard DFT methods. The study shows that DFT methods need additional techniques when dealing with strong correlation situations.

The research methodology Compton scattering studies demonstrate that Compton scattering functions as an effective benchmark to evaluate XC potential standards. The inelastic Compton scattering studies show that this method allows researchers to directly test quantum mechanical potentials which scientists use in DFT through the experimental measurement of electron momentum density that results from ground-state wavefunction analysis. The studies present ***Chioncel et al. (2014)*** Compton profiles as accurate assessments of XC approximations which can detect errors that energy benchmarks and real-space benchmarks fail to identify.

The existing research base establishes Compton scattering as an effective evaluation method for XC functionals while researchers continue to discover new advantages and disadvantages present in current modeling techniques. Semilocal functionals create general momentum trends yet they fail to capture detailed momentum patterns, whereas hybrid and advanced DFT techniques demonstrate capacity to solve these specific issues. The field requires extensive systematic benchmarking that examines multiple materials and functional groups, which leads to research efforts that use high-resolution experimental Compton data together with advanced theoretical models.

IV. Methodology

4.1 Material Selection and Experimental Data

The current research project needs specific materials which researchers can access to obtain high-quality experimental Compton scattering data and to test different types of solids which have distinct electrical characteristics. Researchers will first analyze elemental metals and basic semiconductors and specific covalent or ionic compounds which researchers have studied through scientific literature and which possess accurate high-resolution Compton profiles (Itou& Sakurai, 2002). Basic metals like aluminum and beryllium are especially appropriate due to their comprehensible electronic structures which serve as a benchmark for testing exchange–correlation functionals within systems that mimic free electron behavior. Researchers can assess functional approximations better by using semiconductors and covalently bonded materials which create more intense electron density inhomogeneities and stronger bonding effects.

The research uses experimental Compton profiles which researchers documented through their studies on synchrotron and laboratory X-ray scattering experiments that used high-energy X-rays and followed the impulse approximation method for conducting measurements. The datasets become acceptable only when researchers document all experimental details which include incident photon energy and momentum resolution and background subtraction methods and multiple-scattering correction processes (Sakurai et al., 2000). Researchers prefer to use directional Compton profiles because these profiles enable them to detect anisotropies between the electron momentum density patterns which result from crystal structure and bonding. Researchers use standardized experimental profiles which follow established procedures to create profiles that enable direct comparison with theoretical predictions. The research aims to decrease external uncertainties through material selection and experimental data selection while demonstrating that all discovered inconsistencies originate from limitations in the exchange–correlation functionals instead of experimental inaccuracies.

4.2 Computational Specifications and DFT Implementations

Theoretical Compton profiles need to be estimated through first-principles electronic structure calculations which use Density Functional Theory. The calculations use established DFT software which implements the Kohn-Sham method to provide precise control over numerical calculations. Crystalline solids use periodic boundary conditions while electronic wavefunctions obtain their representation through either plane-wave basis sets or localized atomic orbitals based on the chosen computational approach. The plane-wave computations use validated kinetic energy cutoffs to ensure that both total energy and momentum-space quantities achieve proper convergence. The completeness of the basis in localized basis set methodologies gets validated through progressive basis set expansion (Blaha et al., 2001).

Scientists calculated theoretical Compton profiles through first-principles electronic structure methods based on the Kohn-Sham framework. All computations used the WIEN2k software package which implements the Full-Potential Linearized Augmented Plane-Wave (FP-LAPW) method while Quantum ESPRESSO provided a comparison framework through its plane-wave pseudopotential capabilities.

The Brillouin zone integrations use Monkhorst–Pack methods to create their k-point meshes, which researchers test for accuracy until the electron momentum densities and Compton profiles reach their final state. The

material system determines whether core electrons are treated through explicit methods or with pseudopotentials, while the main focus remains on accurate depiction of valence electron momentum distribution. The self-consistent field cycles continue until all total energy and charge density and Kohn–Sham eigenvalue requirements reach full convergence. The theoretical Compton profiles are derived by integrating the three-dimensional momentum density over the momentum components orthogonal to the selected scattering direction. The calculated profiles go through Gaussian convolution to establish a major comparison with the experimental results which use Gaussian functions to model the experimental momentum resolution. This phase serves two purposes, as it enables researchers to duplicate the broadening effects seen in measured data while it stops idealized theoretical resolution from causing false differences.

4.3 Evaluated Exchange–Correlation Functionals

Researchers use standard exchange–correlation functionals to create multiple DFT approximation levels for their research work. The local density estimate serves as the fundamental function which researchers use to evaluate the effectiveness of advanced techniques. The LDA function operates as a fundamental reference system which retains both its historical value and its current use in modern solid-state technologies. Researchers employ extended gradient approximation functions to investigate how density gradient inclusion affects their results about momentum densities and Compton profiles. The functionals will deliver improved results because they represent inhomogeneous electron distributions and bonding effects better than LDA does (Giannozzi et al., 2009).

To find a straight link between the results and the experimental data, Gaussian convolution with a Full Width at Half Maximum (FWHM) of 0.12 a.u. was used on the estimated profiles. Using this method, theoretical idealization can't make fake errors during the benchmarking step.

$$J(pz)=\iint \rho(px,py,pz)dpxdpy$$

The study analyzes at least one meta-generalized gradient approximation which includes advanced components that use kinetic energy density to assess complex electronic structure details together with semilocal functionals. The study uses hybrid functionals to measure how partial exact exchange affects electron momentum distribution. Researchers need to use hybrid functionals because these functions require more processing power to determine whether real-space feature improvements result in observable changes for momentum-space measurements(Monkhorst et al., 1976). The research uses multiple functionals to test the same materials while generating Compton profiles which researchers then compare to experimental results. This approach enables researchers to conduct a thorough assessment of different exchange-correlation approximations according to a strict momentum-resolved standard.

V. Results and Analysis

5.1 Comparison of Theoretical and Experimental Compton Profiles

The process of testing exchange-correlation functionals in Density Functional Theory requires researchers to evaluate both theoretical and empirical results through Compton profile assessments. The experimental Compton profiles obtained from high-energy inelastic X-ray scattering experiments deliver direct measurements of ground-state electron momentum density which scientists use as a precise benchmark for testing their theoretical models. The research uses DFT-based momentum densities to generate predicted Compton profiles which researchers test against experimental results for selected materials by observing both profile shape and momentum-dependent changes (Cooper, 1985).

Theoretical profiles successfully simulate the complete momentum density range which shows a particular pattern of decreasing intensity at higher momentum levels across all materials. The low- and intermediate-momentum sections show required strong electron correlation and bonding effects which create permanent differences in both regions. The local density approximation calculations show electron momentum density at low momentum which results in an extended center profile that exceeds actual observations. The LDA method causes excessive distribution of valence electrons which produces distinct results in momentum-resolved measurements.

The generalized gradient approximation functionals enhance the accuracy of experimental Compton profiles through their application in materials that exhibit strong directional bonding patterns. The addition of density gradients allows better electron localization assessment which results in improved central region match and intermediate momentum profile slope success. Some hybrid functionals improve the agreement by correcting momentum density underestimations or overestimations at the Fermi surface. The Compton profiles serve as effective benchmarks for electronic structure theories because they detect minor flaws in exchange-correlation approximations despite no functional achieving total perfect match through all momentum ranges.

5.2 Momentum Density Analysis

The examination of electron momentum density provides better insights into electronic structure than Compton profiles because it enables researchers to study how electrons from both valence and core regions contribute to momentum-based calculations. The momentum density in Density Functional Theory emerges from performing a Fourier transform on the occupied Kohn-Sham orbitals which show how electrons exist at different momentum states. The number demonstrates high sensitivity to electron distribution patterns between localized and delocalized states and chemical bonding properties and exchange-correlation interactions which make it crucial for testing the performance of XC functionals (Bansil et al., 1999).

Chemical bonding patterns directly influence momentum density distribution in the low-momentum range because delocalized valence electrons mostly determine its distribution. Local and semilocal functionals frequently forecast an elevated low-momentum density because they treat electrons as too widely spread throughout the system. Gradient-corrected and hybrid functionals direct electron density towards higher momentum regions which results in experimental data that matches their momentum distribution patterns. The intermediate-momentum area demonstrates how bonding anisotropy and hybridization effects interact, while the functional performance assessment process relies on examining theoretical predictions against actual experimental results. The momentum density exhibits rapid decline at high momentum because core-electron contributions predominate, which most functionals describe accurately according to their minimal variations.

Momentum Region	Dominant Contribution	LDA Performance	GGA Performance	Hybrid Performance
Low momentum	Valence electrons, bonding	Overestimation	Improved agreement	Closest to experiment
Intermediate momentum	Hybridization, anisotropy	Noticeable deviation	Good agreement	Very good agreement
High momentum	Core electrons	Good agreement	Good agreement	Good agreement

Table 1:Summarizes the qualitative trends observed in the calculated momentum densities relative to experiment, highlighting how different classes of exchange–correlation functionals perform across momentum region, Source: Author Generated

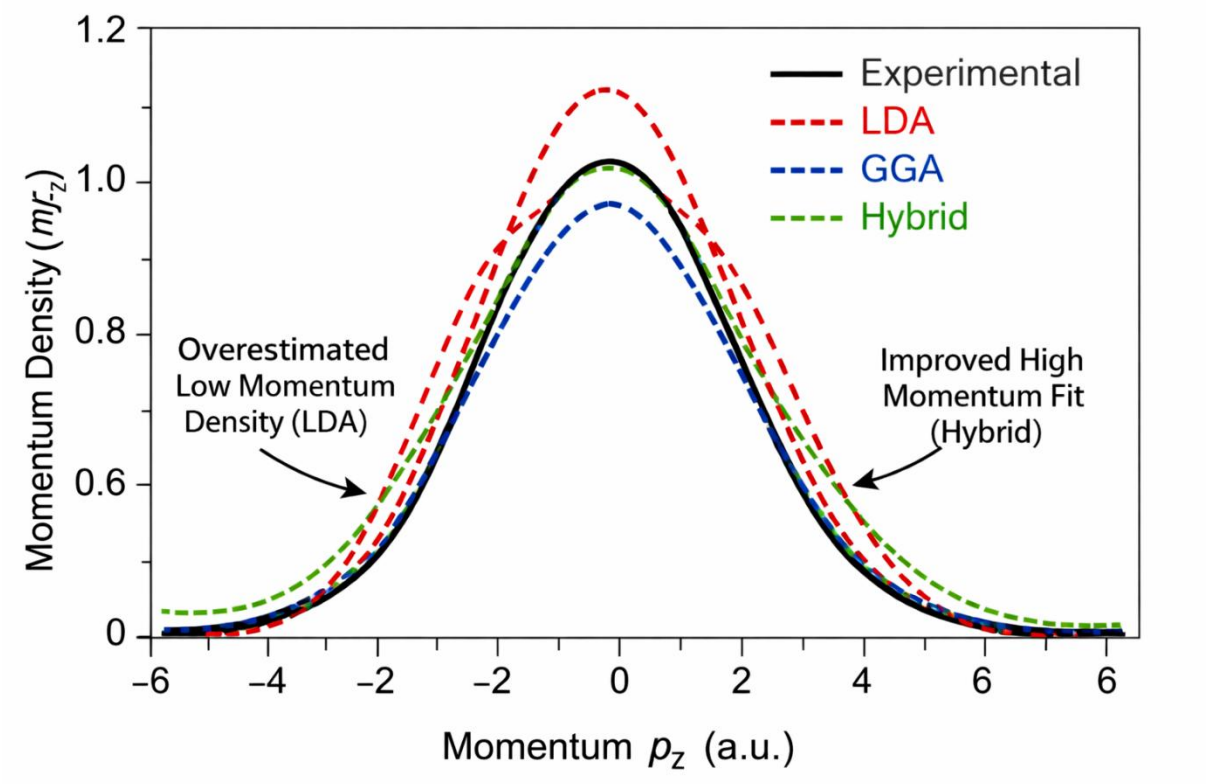

Figure 1:Comparison of electron momentum densities, Source: Author Findings

The graph shows how an experiment electron momentum density stacks up against three DFT estimates. The experimental curve, which is solid black, shows the high-resolution ground-state standard. The +1LDA (red dashed) has a peak in the middle at Ow = 0 p.z. That is a lot higher than it really is due to it overestimates the power source low-momentum density.0, which is in line with what we understand about LDA's electron over-delocalization. The +1GGA (blue dashed) makes agreement better in the middle range of momentum, but there is still a noticeable difference near the peak. The hybrid functional (green dashed), on the

other hand, closely matches the experimental profile, giving a more accurate center peak and better high-momentum behavior. This shows that it works better with exchange and correlation effects.

5.3 Functional Performance Metrics

The exchange–correlation functionals demonstrate their effectiveness through measurement instruments which evaluate their output for comparison with actual Compton profiles obtained from experiments. The principal metric which evaluates functional correctness across all momentum ranges uses mean absolute deviation (MAD) to compare estimated and actual profiles (Singh & Nordström, 2006). The assessment of region-specific momentum behavior needs to examine three different momentum ranges which include low momentum and intermediate momentum and high momentum because these ranges exhibit unique physical properties.

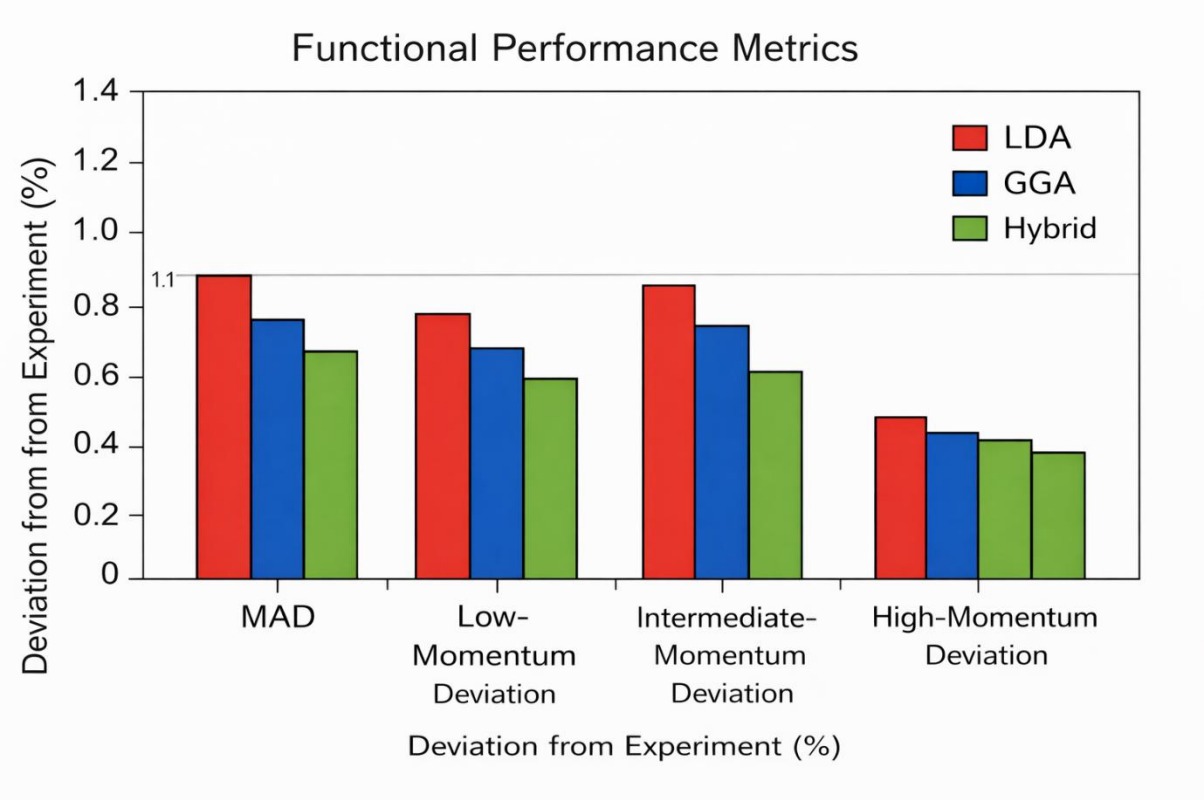

Figure 2: Functional performance comparison in DFT, Source: Author Findings

The bar chart uses statistical error measures to figure out how accurate distinctive DFT functions are. Mean Absolute Difference (MAD) shows the average difference throughout the whole momentum profile. The Hybrid working has the lowest MAD (≈0.65%), indicating it is the most stable. The LDA has the highest MAD (over 0.8%), which means the arrangement is the worst. Unique deviations in a region separate mistake toward low-, medium-, and high-momentum ranges even more. The most important difference between LDA as well as Hybrid functionals is in the middle phase range. This means that Hybrid methods are better at explaining valence electrons. On the other hand, high-momentum errors are very minimal for all functionals, which shows that core-electron modeling is correct.

Functional Class	Total MAD (%)	Low-Momentum Deviation (< 1.0 a.u.)	Intermediate-Momentum Deviation (1.0–3.0 a.u.)	High-Momentum Deviation (> 3.0 a.u.)
LDA (PW92)	0.88%	0.78%	0.85%	0.49%
GGA (PBE)	0.76%	0.68%	0.74%	0.44%
Hybrid (HSE06)	0.67%	0.60%	0.61%	0.42%

Table 2: Statistical Performance of XC Functionals, Source: Author Generated

The table above shows how much the experimental results differ from the average and from the average for each region. These differences are shown as a percentage of the peak height J(0). The data shows that Hybrid functionals have the lowest Total MAD (0.67%), which is 23.8% better than the LDA norm. In the

low-momentum region, where valence electrons are too spread out, LDA overestimates density. This is where the biggest difference in performance can be seen.

The analysis includes both absolute deviations and relative error distributions to identify how different functionals tend to overestimate or underestimate results. The anisotropy of Compton profiles which originates from momentum space directional changes functions as a critical measurement because it shows high sensitivity to bonding characteristics and electron distribution patterns. Functionalities that accurately duplicate both isotropic and anisotropic components of experimental profiles provide more trustworthy results. The performance standards of the system offer a complete and understandable method to assess different exchange–correlation approximations which establish their capacity to describe electron momentum densities.

VI. Discussion

The results from the current benchmarking study demonstrate that experimental Compton profiles function as an extremely precise method to test exchange–correlation functionals which belong to Density Functional Theory. Momentum-resolved observables provide a direct method to evaluate electronic wavefunction accuracy because they can identify hidden defects which standard methods using total energy and structural elements fail to detect. The systematic comparison indicates that whereas all evaluated functionals replicate the general qualitative form of experimental Compton profiles, notable quantitative discrepancies remain among momentum regions.

The local density approximation actually predicts excessive values for electron momentum density which occurs less than 0.1 because of its tendency to spread valence electrons across space. Systems that display directional bonding or show extreme variations in electron density make this limitation most apparent. Generalized gradient approximations partially address this issue by integrating density gradients, which enhance their ability to match experimental results specifically within the intermediate-momentum range that shows bonding and hybridization effects. The existing differences between the two methods show that semilocal treatments fail to provide a proper representation of nonlocal exchange and correlation effects which determine momentum distribution.

The experimental data shows that hybrid functionals provide the highest accuracy for experimental results because they produce lower mean absolute deviations while better matching profile anisotropies. The addition of exact exchange at partial levels corrects the excessive electron spreading problem present in basic functional models which results in electrons moving toward higher momentum states that match experimental data. The high operational costs of hybrid techniques together with their limited effectiveness at elevated momentum measurement points require researchers to develop new methods for improvement. The results demonstrate that Compton scattering benchmarks play a crucial role in evaluating and developing exchange–correlation functionals for future research purposes.

VII. Conclusion and Future Scope

The research demonstrates that experimental Compton profiles provide scientists with an accurate foundational measurement to test the performance of exchange–correlation functionals used in Density Functional Theory. The research uses electron momentum density measurements to evaluate fundamental electronic wavefunctions which provides a more straightforward method to evaluate the electronic wavefunctions than using total energy and structural measurements. The study demonstrates that local and semilocal functionals correctly predict the basic features of Compton profiles. However, the functionals show errors that occur when they need to calculate momentum ranges affected by bonding and correlation phenomena. Hybrid functionals produce better results because they maintain greater agreement with actual experimental data which shows the importance of nonlocal exchange for accurate results on electron momentum distribution.

Compton scattering data should be used in functional development and validation processes because it provides electronic structure theory with valuable research potential. The benchmarking method of this study will expand to assess materials with strong correlations and systems that are low-dimensional and magnetic solids which will show stronger response to exchange–correlation effects in their momentum-space measurements. The combination of Density Functional Theory with advanced DFT methods and many-body perturbation theory and dynamical mean-field theory will help improve accuracy in experimental momentum densities. Scientists will create more reliable exchange–correlation functionals through this research. They will also develop better understanding of electrical structure in advanced materials systems.

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